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Corrosion inhibition of 7150 Al alloy in the presence of some amino acids – molecular dynamics simulation, quantum chemical, and electrochemical studies

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ABSTRACT

Inhibition performance of three amino acids, namely L-phenylalanine (Phe), L-methionine (Met), and L-histidine (His) as corrosion inhibitors for 7150 Al alloy surface in 0.1M HCl + 1M NaCl solution was investigated using cyclic polarization test, quantum chemistry calculation, and molecular dynamics (MD) simulation. A significant decrease in the corrosion rate of alloy was observed in the presence of the amino acids. The inhibition efficiency is in the following decreasing order under all studied temperatures: Phe < Met < His, as revealed by the electrochemical results. From the calculated binding energies by MD, His shows preferred adsorption on the alloy surface among the three tested amino acids, showing good consistent with electrochemical data. Quantum chemistry calculations were performed under water–metal interface conditions with dielectric constant equals 6. The results showed that quantum chemistry parameters such as dipole moment values, E_{HOMO}, and $E_{LUMO} - E_{HOMO}$ might not be able to show good agreement with experimental inhibition efficiency. However, the adsorption sites of the studied inhibitors can be determined using Fukui indices and Mulliken charges of the local atoms, as calculated through quantum chemistry method.

KEYWORDS: 7150 Al alloy, amino acids, corrosion inhibition, quantum chemistry, molecular dynamics, cyclic polarization